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TITLE: Alcohols selective aminations: A DFT based micro-kinetics modelling strategy for screening the promising heterogeneous catalysts
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ABSTRACT BODY:
Abstract: Amines are useful intermediates in the bulk and fine chemical industries. However, current industrial synthesis of them requires the application or production of toxic compounds and relies on the limited petroleum feedstock. Recently, the alkylation of amines with alcohols obtained from renewable resources to give higher order amines has proven to be an attractive and environmentally friendly alternative synthesis methods, which relies on a heterogeneous catalyst to be efficient. Despite of the extensive experimental and theoretical investigations for this type of reaction on different metals, it is obviously not practical and also not efficient to test every catalyst by either experimental or theoretical tools without any guidelines. Therefore, it would be very interesting and useful if there are some structure-activity or simply descriptor-activity relations either from experimental or theoretical that can guide the choice and design of new catalyst for this type of reaction. To provide the guideline for screening potential catalyst, we present a combination of experimental and DFT-PBE-dDsC based micro-kinetics modeling investigations of alcohol selective amination process on the close packed surface of nine transition metals. Our strategy is to build an experimentally verified activity – simple descriptor relation to efficiently screen different types of catalysts, and finally provide important reference for the experimental design and finding of promising catalysts for alcohol selective amination.
(No Image Selected)